Parallel Rate Matrix Solvers in the ATOMIC Code

James Colgan and Joseph Abdallah (T-4), Christopher J. Fontes and H. L. Zhang (X-5)

The need to solve large systems of equations in order to model non-Local Thermodynamic Equilibrium (non-LTE) plasmas is becoming increasingly important. Los Alamos National Laboratory (LANL) data were submitted to the recent NLTE-3 workshop in Gaithersburg, Maryland, where comparisons were carried out among a number of international modeling efforts [1]. In some of the test cases the largest models predicted significantly different plasma behavior when compared to results from smaller models. Another use of non-LTE data involves the attempt to create an in-line, rad-hydro algorithm for computing non-LTE atomic spectra via the effective rate method [2], which requires tables of accurate atomic data. For LTE plasmas, the tabular data approach has been in use for many years. However, the concept is relatively unexplored for non-LTE modeling for a number of reasons, as discussed in [2]. One of the reasons for this disparity is the need to solve a system of coupled rate equations in order to obtain the atomic level populations in the non-LTE case. For LTE plasmas the populations can be obtained from the much simpler Saha equation.

For heavy elements, the LANL suite of codes regularly calculates models containing on the order of 100,000 relativistic configurations. However, in order to move beyond models of this size a more efficient method of solving the rate equations is needed because the amount of computing time and memory quickly becomes prohibitive as the number of configurations is increased.

Currently the LANL code ATOMIC contains two rate matrix solvers, which are only able to run in a serial manner. The first (direct) solver performs the solution using standard LU decomposition techniques designed for a general matrix. This solver is typically very stable; however, the time to run the solver scales as around n^3 (n being the number of configurations), and also the memory required to store the rate matrix quickly becomes prohibitively large. Therefore this solver has only been used for relatively small problem sizes to date. The second rate matrix solver in ATOMIC is an incomplete LU iterative sparse solver. This solver has been found to run very quickly for larger problems. Problems containing up to around 300,000 configurations have already been solved using this method. However, the stability of more ill-conditioned problems (e.g., those containing neutral ion stages) is sometimes uncertain. Also, in order to move to larger configuration data sets, the memory required to hold the data becomes progressively larger and needs to be distributed over several processors to fit on current machines.

Although three different types of parallel rate matrix solvers were considered, here we focus on the LAMG solver, developed at LANL. This package has been the subject of a previous LANL memo [3]. This code has previously been demonstrated to give scalable performance on shared and distributed-memory parallel platforms.

At the present time, this code has solved problems on the order of 1.2 million configurations [4]. The solver scales well for up to 128 processors on the LANL QSC machine. The run-time requirements of the solver, when 128 processors are used, are comparable to the iterative sparse serial solver. The code has been checked and modified where necessary to ensure that as little memory as possible is used throughout the code. This becomes very important, since the input data sets which generate up to 1 million or more configurations typically require arrays which use greater than 10.0 Gb of RAM memory. Figure 1 shows three different emissivity calculations for a Xe spectrum, where models containing different numbers of configurations are shown. For this electron temperature (200 eV) and density ($1.1 \times 10^{20}/\mathrm{cm}^3$) we find that the spectrum appears to be reasonably well converged with respect to the number of configurations included in the model. Also, the radiative power loss from the largest

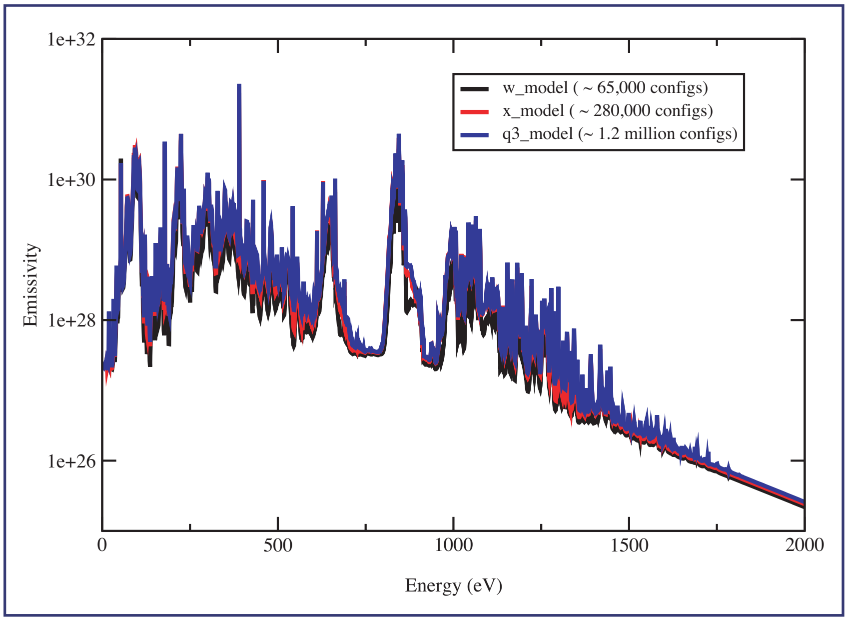

***Figure 1—* Xenon emissivities for three ATOMIC models at an electron temperature of 200 eV and an electron density of $1.1 \times 10^{20}/cm^3$.**

model is within 4% of the smaller model. Further efforts are underway to compare such spectra to experimental results.

We find that parallel rate matrix solvers have been demonstrated to extend the size of the rate matrices that can be calculated by the ATOMIC code. We have demonstrated that the current parallel iterative sparse rate matrix solvers can solve systems containing on the order of 1 million configurations. This work, along with other advances in the ATOMIC package, should make significant progress towards the goals of non-LTE atomic data table generation and improved agreement when comparing with experimental data.

[1] C.J. Fontes, et al., "LANL Data Submissions to the NLTE-3 Workshop," Los Alamos National Laboratory memorandum X-5:04-49 (U) (June 2004).
[2] C.J. Fontes, et al., *J. Quant. Spectros. Rad. Transfer* **65**, 223 (2000).
[3] "LAMG: Los Alamos Multigrid Code Reference Manual," Los Alamos National Laboratory report LA-UR-03-6183 (December 2003).
[4] J. Colgan and C.J. Fontes, "Parallel Rate Matrix Solvers in the ATOMIC code," Los Alamos National Laboratory memorandum X-5:04-48 (U) (July 2004)

For more information, contact James Colgan (jcolgan@lanl.gov).

Acknowledgements
We would like to acknowledge NNSA's Advanced Simulation and Computing (ASC), Materials and Physics Program for financial support.